

Tetrachlorophthalic acid
632-58-6 | DTXSID6060896

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 9.44e-02 mol/L

Global applicability domain: Inside

Local applicability domain index: 3.84e-01

Confidence level: 6.57e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>[(carboxymethyl)sulfanyl] (phenyl)acetic acid</div> <div>Measured: 6.98e-02</div> <div>Predicted: 9.49e-02</div>	<div>Image not found</div> <div>2,2'-tetrasulfane-1,4-diyl diacetic acid</div> <div>Measured: 3.53e-02</div> <div>Predicted: 4.92e-02</div>	<div>Image not found</div> <div>3,3'-Dithiodipropionic acid</div> <div>Measured: 6.39e-01</div> <div>Predicted: 2.87e-01</div>
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